

Isopropyl butyrate

Other names:	1-Methylethyl butanoate 2-Propyl butanoate Butanoic acid, 1-methylethyl ester Butyric acid, isopropyl ester Isopropyl butanoate Isopropyl n-butyrate UN 2405 n-Butyric acid isopropyl ester n-C3H7C(O)OCH(CH3)2
Inchi:	InChI=1S/C7H14O2/c1-4-5-7(8)9-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	FFOPEPMHKILNIT-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCC(=O)OC(C)C
Mol. weight [g/mol]:	130.18
CAS:	638-11-9

Physical Properties

Property code	Value	Unit	Source
chl	-4184.40	kJ/mol	NIST Webbook
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.738		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	842.00		NIST Webbook

rinpol	855.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	848.00	NIST Webbook
rinpol	823.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	843.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	834.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	847.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	828.00	NIST Webbook
rinpol	842.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	814.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	827.60	NIST Webbook
ripol	1051.00	NIST Webbook
ripol	1043.00	NIST Webbook
ripol	1030.00	NIST Webbook
ripol	1042.00	NIST Webbook
ripol	1028.00	NIST Webbook
ripol	1030.00	NIST Webbook
ripol	1028.00	NIST Webbook
ripol	1090.00	NIST Webbook
ripol	1060.00	NIST Webbook
ripol	1058.00	NIST Webbook
ripol	1036.00	NIST Webbook
ripol	1050.00	NIST Webbook
ripol	1043.00	NIST Webbook
ripol	1024.00	NIST Webbook
ripol	1039.00	NIST Webbook
ripol	1046.00	NIST Webbook

tb	403.70	K	NIST Webbook
tb	403.45 ± 2.00	K	NIST Webbook
tb	401.15 ± 1.00	K	NIST Webbook
tb	404.65 ± 1.00	K	NIST Webbook
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0047724	Paxs	225.81	Joback Method
dvisc	0.0021099	Paxs	260.74	Joback Method
dvisc	0.0011312	Paxs	295.68	Joback Method
dvisc	0.0006919	Paxs	330.61	Joback Method
dvisc	0.0004649	Paxs	365.54	Joback Method
dvisc	0.0003348	Paxs	400.48	Joback Method
dvisc	0.0002542	Paxs	435.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49071e+01
Coeff. B	-3.60451e+03
Coeff. C	-5.33650e+01
Temperature range (K), min.	299.92
Temperature range (K), max.	429.01

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638119&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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